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Pair interaction model based Kinetic Monte Carlo simulation of oxygen and metal diffusion in Ni-based alloys DOMINIC ALFONSO, National Energy Technology Laboratory - Department of Energy, DENYAGO TAFEN, National Energy Technology Laboratory, COMPUTATIONAL FUNCTIONAL MATERIALS TEAM — Investigation of oxygen and metal diffusion processes in Ni-based alloy is a problem of high relevance in the area of understanding corrosion behavior. We explored the use of combined approach consisting of density functional theory to compute migration barriers and kinetic Monte Carlo method to evaluate long-time diffusivities of oxygen and metals in Ni containing Al and Fe. Pair interaction model was used to evaluate the influence of the local environment on the kinetic parameters. For reference, vacancy mediated self-diffusion in pure Ni was examined. A diffusion prefactor and barrier of Do = 2.4 x 10^{-5} m^2/sec and Q =2.90 eV were predicted in very good agreement with experimental values of 9.8 x 10^{-5} m^2/sec and Q =2.88 eV. Results for (i) Al impurity, (ii) Fe impurity and (iii) concentrated Fe diffusion exhibit good agreement with available experimental data. The model was employed for oxygen diffusion in Ni and it was found that the inclusion of vacancy improves the level of agreement with compilation of experimental studies. The presence of either Al or Fe reduces the diffusivity of oxygen. This was attributed to the increase in the excess energy of oxygen in Ni due to these metals.

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